

10797038 9/28/06

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:09:51 ON 29 SEP 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:10:02 ON 29 SEP 2006

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STRUCTURE FILE UPDATES: 27 SEP 2006 HIGHEST RN 909000-49-3

DICTIONARY FILE UPDATES: 27 SEP 2006 HIGHEST RN 909000-49-3

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

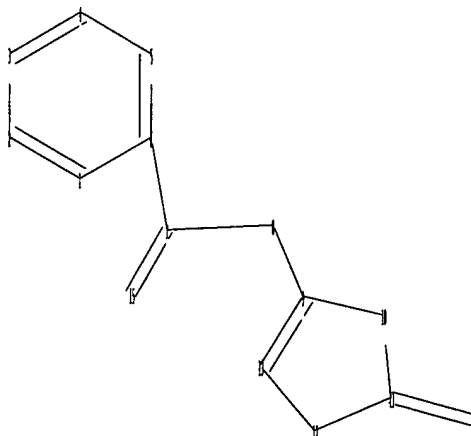
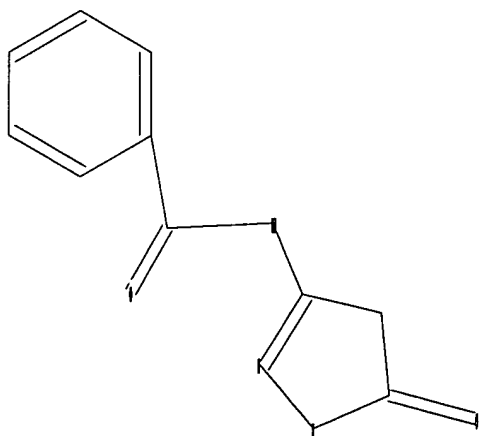
Please note that search-term pricing does apply when conducting SmartSELECT searches.

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<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10797038.str



chain nodes :

7 8 14 15

ring nodes :

1 2 3 4 5 6 9 10 11 12 13

10797038 9/28/06

chain bonds :

6-7 7-8 7-15 8-9 11-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13

exact/norm bonds :

7-8 7-15 8-9 9-13 11-12 11-14 12-13

exact bonds :

6-7 9-10 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 9 :

Match level :

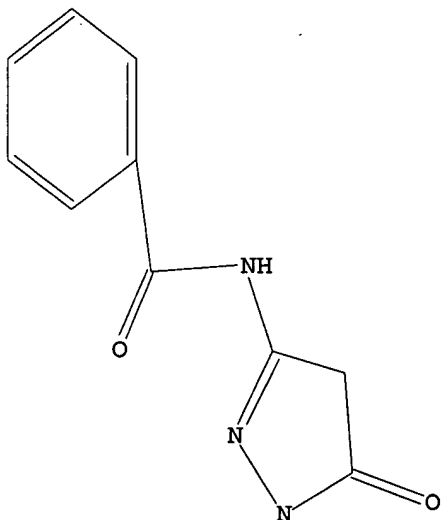
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:10:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 116 TO ITERATE

100.0% PROCESSED 116 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

10797038 9/28/06

BATCH **COMPLETE**
PROJECTED ITERATIONS: 1674 TO 2966
PROJECTED ANSWERS: 1265 TO 2415

L2 50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 10:12:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2436 TO ITERATE

100.0% PROCESSED 2436 ITERATIONS 1950 ANSWERS
SEARCH TIME: 00.00.05

L3 1950 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 168.70 168.91

FILE 'CAPLUS' ENTERED AT 10:12:50 ON 29 SEP 2006
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FILE COVERS 1907 - 29 Sep 2006 VOL 145 ISS 15
FILE LAST UPDATED: 28 Sep 2006 (20060928/ED)

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=> s l3 and barium
1144 L3
247945 BARIUM
12 BARIUMS
247947 BARIUM
(BARIUM OR BARIUMS)

L4 4 L3 AND BARIUM

=> d ibib abs histr tot
'HISTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI

BIB ----- AN, plus Bibliographic Data and PI table (default)
 CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
 CLASS ----- IPC, NCL, ECLA, FTERM
 DALL ----- ALL, delimited (end of each field identified)
 DMAX ----- MAX, delimited for post-processing
 FAM ----- AN, PI and PRAI in table, plus Patent Family data
 FBIB ----- AN, BIB, plus Patent FAM
 IND ----- Indexing data
 IPC ----- International Patent Classifications
 MAX ----- ALL, plus Patent FAM, RE
 PATS ----- PI, SO
 SAM ----- CC, SX, TI, ST, IT
 SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
 SCAN must be entered on the same line as the DISPLAY,
 e.g., D SCAN or DISPLAY SCAN)
 STD ----- BIB, CLASS

 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IMAX ----- MAX, indented with text labels
 ISTD ----- STD, indented with text labels

 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 HIT ----- Fields containing hit terms
 HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
 containing hit terms
 HITRN ----- HIT RN and its text modification
 HITSTR ----- HIT RN, its text modification, its CA index name, and
 its structure diagram
 HITSEQ ----- HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 FHITSTR ----- First HIT RN, its text modification, its CA index name, and
 its structure diagram
 FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 KWIC ----- Hit term plus 20 words on either side
 OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

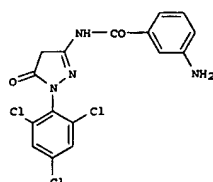
All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
 ENTER DISPLAY FORMAT (BIB):end

=> d ibib abs hitstr tot

10797038 9/28/06

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

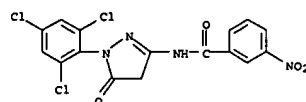
ACCESSION NUMBER: 2005:495149 CAPLUS
DOCUMENT NUMBER: 144:232961
TITLE: Synthesis of 3-(3'-aminobenzoylamido)-1-(2',4',6'-trichlorophenyl)pyrazol-5-one, an intermediate in the synthesis of the purple component of color photographic materials
AUTHOR(S): Yuttilov, Yu. M.; Smolyar, N. N.; Minkina, L. V.
CORPORATE SOURCE: Litvinenko Institute of Physical Organic and Coal Chemistry, National Academy of Sciences of Ukraine, Donetsk, Ukraine
SOURCE: Russian Journal of Applied Chemistry (2005), 78(2), 278-280
CODEN: RJACEO; ISSN: 1070-4272
PUBLISHER: Pleiades Publishing, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



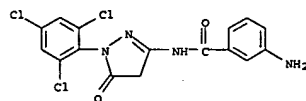
I

AB Catalytic reduction of 3-(3'-nitrobenzoylamido)-1-(2',4',6'-trichlorophenyl)pyrazol-5-one with hydrogen and hydrazine hydrate to 3-(3'-aminobenzoylamido)-1-(2',4',6'-trichlorophenyl)pyrazol-5-one (I), the key intermediate in the synthesis of the purple component of color photog. and motion picture materials, was studied.
IT 63134-25-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (aminobenzoylamido)(trichlorophenyl)pyrazolone via reduction of its nitrobenzoyl analog by hydrogen or hydrazine catalyzed by Group 10 metal catalysts)
RN 63134-25-8 CAPLUS
CN Benzamide, N-[4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-pyrazol-3-yl]-3-nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 40567-18-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (aminobenzoylamido)(trichlorophenyl)pyrazolone via reduction of its nitrobenzoyl analog by hydrogen or hydrazine catalyzed by Group 10 metal catalysts)
RN 40567-18-8 CAPLUS
CN Benzamide, 3-amino-N-[4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



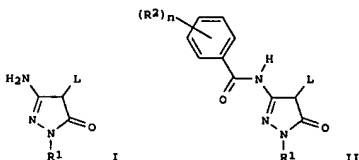
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:819915 CAPLUS
DOCUMENT NUMBER: 141:296015
TITLE: Preparation of 3-amino-4-substituted-5-pyrazolones
INVENTOR(S): Mori, Hideto
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKKXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

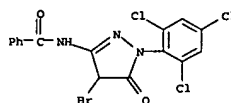
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004277331	A2	20041007	JP 2003-70179	20030314
US 2004204589	A1	20041014	US 2004-797038	20040311
PRIORITY APPLN. INFO.			JP 2003-70179	A 20030314

OTHER SOURCE(S): CASREACT 141:296015; MARPAT 141:296015
GI

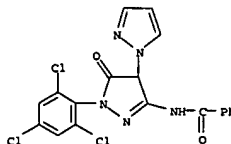


AB The pyrazolones I (R1 = alkyl, aryl; L = thiocyno, aryloxy, alkoxy, etc.) as intermediates for polymer photog. couplers are manufactured by hydrolysis of benzoylamino-pyrazolones II (R1, L = same as I; R2 = substituent; n = 0-5) in the presence of Ba compds. and alkali metal hydroxides, precipitation of the Ba compds. as halides, and removal of the halides. Thus, II (R1 = 2,4,6-trichlorophenyl, R2 = H) was hydrolyzed in the presence of Ba(OH)2 and NaOH in MeOH, HCl added, filtered to remove BaCl2 and NaCl, and extracted with PhMe to remove impurities. The residual aqueous solution was neutralized with NaOH to give 70.5% I (R1 = 2,4,6-trichlorophenyl, R2 = H).
IT 112118-39-5 112118-41-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminopyrazolones by hydrolysis of benzoylamino-pyrazolones in the presence of Ba compds. and alkali metal hydroxides, and precipitation of the Ba compds. as halides)
RN 112118-39-5 CAPLUS
CN Benzamide, N-[4-bromo-4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
pyrazol-3-yl]- (9CI) (CA INDEX NAME)



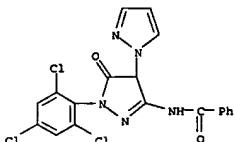
RN 112118-41-9 CAPLUS
CN Benzamide, N-[4',5'-dihydro-5'-oxo-1'-(2,4,6-trichlorophenyl)[1,4'-bi-1H-pyrazol]-3'-yl]- (9CI) (CA INDEX NAME)



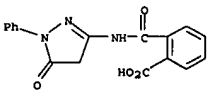
L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2002:900799 CAPLUS
 DOCUMENT NUMBER: 138:4596
 TITLE: Preparation of 3-amino-4-substituted-5-pyrazolones
 INVENTOR(S): Suzuki, Akira; Yamakawa, Kazuyoshi
 PATENT ASSIGNER(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAP
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002338548	A2	20021127	JP 2001-149314	20010518
PRIORITY APPLN. INFO.: JP 2001-149314 20010518				

OTHER SOURCE(S): CASREACT 138:4596; MARPAT 138:4596
 AB The title compds., useful as intermediates for polymer couplers, etc., are prepared by hydrolyzing 4-substituted-5-pyrazolones containing (un)substituted benzoylamino group at 3-position with alkalis, e.g. Ba or Li compds. 3-Benzoylamino-4-(1-pyrazolyl)-1-(2,4,6-trichlorophenyl)-5-pyrazolone was treated with Ba(OH)2 in MeOH at 65° for 6 h to give 91.1% 3-amino-4-(1-pyrazolyl)-1-(2,4,6-trichlorophenyl)-5-pyrazolone (I). A photocog. material containing a polymer coupler, prepared from I showed lower fog than a control material using polymer coupler derived from I prepared by acid hydrolysis.
 IT 112118-41-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 3-aminopyrazolones as intermediates for polymer couplers by alkali hydrolysis of N-benzoylamino derivs.)
 RN 112118-41-9 CAPLUS
 CN Benzamide, N-[4',5'-dihydro-5'-oxo-1'-(2,4,6-trichlorophenyl)-1,4'-bi-1H-pyrazol-3'-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 yielded EtOCH2CONH2, needles from PhH, m. 80-2° (cf. Sommelet, Ann. chim. phys. [8] 9, 493). One mol. of EtOCH2COCH:NOH reacting with 1 mol. of o-C6H4(NH2)2 in 2 mols. of glacial AcOH gave rise to 2-ethoxymethylquinoxaline (H), CH:N.C6H4.N:CH2OEt, b13 144°, neutral to litmus in aq. soln.; chloroplatinate, microcrystals, decomp. 250°; picrate, yellow powder, m. 216°. Upon gradual oxidation with alk. KMnO4, (A) yielded pyrazine-2,5,6-tricarboxylic acid, HO2CC(CO2H).N.CH2C(CO2H).N, silky needles, m. 191° (decomp.), isolated as the barium salt. The normal copper salt forms green microcrystals from aq. MeOH.
 IT 860761-61-1, 5(4)-Pyrazolone, 3-(o-carboxybenzamido)-1-phenyl- (preparation of)
 RN 860761-61-1 CAPLUS
 CN 5(4)-Pyrazolone, 3-(o-carboxybenzamido)-1-phenyl- (1CI) (CA INDEX NAME)



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1915:15638 CAPLUS
 DOCUMENT NUMBER: 9:15638
 ORIGINAL REFERENCE NO.: 9:2517H-1, 2518a-g
 TITLE: Condensation of acid chlorides with the ethyl ester of

(a) cyanoacetic acid, (b) malonic acid, and (c) acetoacetic acid. II. Experiments on ethyl γ-ethoxyacetoacetate
 AUTHOR(S): Bradshaw, John; Stephen, Henry; Weizmann, Charles
 CORPORATE SOURCE: Manchester
 SOURCE: Journal of the Chemical Society, Transactions (1915), 107, 803-13
 CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB cf. C. A. 8, 904. NaCH(CO2Et)2 reacting with o-C6H4(CO)2NHCH2COCl gave rise to ethyl bisphthaliminocetylmalonate (A), [o-C6H4(CO)2NHCH2CO]2C(CO2Et)2, needles, m. 176°. 1-Phenyl-3-phthaliminomethyl-5-pyrazolone, o-C6H4(CO)2NHCH2C:N.NPh.CO.CH2, microcrystals, m. 192° (decomposition), prepared from PhNHNH2 and Et phthaliminoacetoacetate, when hydrolyzed with alc. KOH yielded 1-phenyl-3-phthaliminomethyl-5-pyrazolone (B), yellow powder, m. 164° (decomposition). Et phthaliminoacetylmalonate (C) and PhNHNH2 condensed to form ethyl 1-phenyl-3-phthaliminomethyl-5-pyrazolone-4-carboxylate (D), o-C6H4(CO)2NHCH2C:N.NPh.CO.CHCO2Et, yellow powder, m. 215°, from which the corresponding (impure) phthalimino derivative was obtained. On fusion, the latter evolved CO2 and yielded (B). By warming an excess of PhNHNH2 with (A) in 50% AcOH, a mixture of (D) and phthaliminoacetylphenylhydrazide (E), o-C6H4(CO)2NHCH2CONHNHPh, needles from MeOH, m. 199°, was obtained. (E) was readily formed by condensing o-C6H4(CO)2NHCH2COCl with PhNHNH2. By treating (C) in KOH with NaNO2 and subsequently adding dilute H2SO4, α-hydroxyimino-γ-phthaliminoacetone, o-C6H4(CO)2NHCH2CO.CH:NOH, prisms from PhH, m. 156° (decomposition), was obtained. When Et2NH was gradually added to an ice-cold mixture of 2 mols. EtOCH2COCH2CO2Et and 1 mol. AcH, ethyl ethylidenebis-γ-ethoxyacetoacetate, needles (from MeOH), m. 96°, was formed, which when heated for 20 hrs. with aqueous H2SO4, or preferably when dissolved in an equal volume of PhH and saturated with HCl,

yielded 1-ethoxy-4-methyl-2-ethoxymethylcyclohexen-6-one, b14 157°, possessing a terpene-like odor; semicarbazone, plates, m. 232° (decomposition). EtOCH2COCHMeCO2Et (P), b16 115°, and EtOCH2COCH2CO2Et (Q), b15 124° (cf. Johnson, J. Chemical Society 35, 582), were formed by treating 1 mol. EtOCH2COCH2CO2Et in EtOH with 1 mol. of MeI and EtI, resp. Similar reactions led to the formation of ethyl γ-ethoxy-α-propylacetoacetate, b18 137°, the corresponding α-isopropylacetoacetate, b18 131°, and α-isobutylacetoacetate, b10 128°, MeCH2COCH2OEt, b. 146°, and EtCH2COCH2OEt, b. 167° (cf. B. acte.ehal and Sommelet, Compt. rend. 138, 89), were obtained in poor yield from (P) and (Q), resp., by heating the esters with H2O in sealed tubes at 210° for 1 hr. The other alkylacetoacetates were hydrolyzed in the same way, "acid hydrolysis" being the principal reaction as shown by the titration of the acid formed during the reaction. EtOCH2COCl and NH3 in dry Et2O

10797038 9/28/06

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

24.23

193.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.00

-3.00

STN INTERNATIONAL LOGOFF AT 10:15:08 ON 29 SEP 2006